

On possible superconductivity in the doped ladder compound $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$

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$\text{LaCuO}_{2.5}$ is a system of coupled, two-chain, cuprate ladders which may be doped systematically by Sr substitution. Motivated by the recent synthesis of single crystals, we investigate theoretically the possibility of superconductivity in this compound. We use a model of spin fluctuation-mediated superconductivity, where the pairing potential is strongly peaked at π in the ladder direction. We solve the coupled gap equations on the bonding and antibonding ladder bands to find superconducting solutions across the range of doping, and discuss their relevance to the real material.

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In the search for the microscopic origin of high- T_c superconductivity (HTS), it is essential to understand not only the materials in which it occurs, but also why it fails to occur in certain systems which are ostensibly only marginally different. In this letter we examine the cuprate $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$, a coupled-chain analog of planar $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. The parent compound was at first thought to be a dopable, two-chain spin ladder system [1], but it was later shown [2–5] that interladder coupling in this unfrustrated structure was sufficiently strong to stabilize long-range antiferromagnetic (AF) order.

The first doping experiments [1,6] were on ceramic samples, and found metallic behavior only for relatively high doping values $x \geq 0.2$. No superconductivity was found for any doping, a result attributed to quasi-one-dimensionality (1d) and the unavoidably strong random potential [3]. Recently, Takagi and coworkers [7] have successfully grown single crystals with the fixed composition $x = 0.15$. These show good metallic characteristics, both along and across the ladder direction with anisotropy ratio $\rho_\perp/\rho_\parallel \sim 8$, and residual resistivities as low as $40\mu\Omega\text{cm}^{-1}$. Although the latter value corresponds to a mean free path exceeding 10 ladder unit cells, at least comparable to coherence lengths in cuprates, there was no indication of superconductivity. The subtlety of the HTS phenomenon was further highlighted by the discovery [8] of superconductivity under pressure in a different cuprate ladder system.

The resistivity data [7] appear to support an anisotropic, 3d approach. Here we consider in detail the Fermi surface of $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$, to find out if there are inherent frustrations present which could hinder or prevent a superconducting state with the predominantly d -symmetric character expected in ladders [9]. To this end we use the model of Millis, Monien and Pines (MMP) [10] for superconductivity mediated by AF spin fluctuations, and perform exploratory calculations examining the form of the resulting gap function.

Considering the structure as two-chain ladders along

\hat{z} , with weaker interladder couplings in the transverse directions, we compute tight-binding bands analogous to the bonding and antibonding combinations in an isolated ladder. In Ref. [3], a set of near-neighbor hopping parameters was deduced from a four-band fit to the band structure computed in the local density approximation (LDA) [11]. Using local, Cu-based orbitals ϕ_1 and ϕ_2 on each atom in the reduced unit cell, the Hamiltonian in terms of reciprocal-space wave functions $\phi_\mu(\mathbf{k}) = V^{-1/2} \sum_i \phi_\mu(\mathbf{r}_i) e^{i\mathbf{k} \cdot \mathbf{r}_i}$ ($\mu = 1, 2$) is

$$H_t = (\phi_1^*, \phi_2^*) \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (1)$$

where

$$t_{11} = t_{22} = -2t_z \cos k_z - 2t'_z \cos 2k_z, \quad (2)$$

$$t_{12} = t_{21}^* = -\tilde{t}_a - \tilde{t}_b [e^{ik_x} + e^{ik_y}], \quad (3)$$

\tilde{t}_i denotes $t_i + 2t'_i \cos k_z$, the ladder lattice constant a_c has been set to 1, and the parameters t_i , shown in Fig. 1, have the values [3] $t_z = t_a = t = 0.4\text{eV}$, $t'_z = \frac{1}{6}t_z$, $t'_a = -\frac{1}{5}t_a$, $t_b = \frac{2}{5}t_a$ and $t'_b = \frac{1}{5}t_b$.

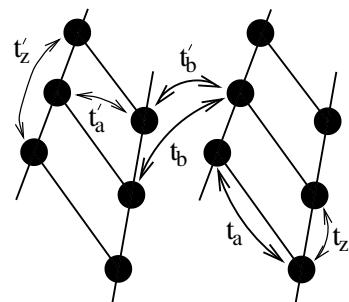


FIG. 1. Two-chain ladder structure of Cu ions in $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$, showing tight-binding parameters.

The two eigenmodes are $\epsilon_{\mathbf{k}\pm} = t_{11}(\mathbf{k}) \pm |t_{12}(\mathbf{k})|$. The nature of the corresponding eigenfunctions is seen most clearly by introducing the bonding and antibonding basis

functions $\phi_{b,a}(\mathbf{k}) = [\phi_1(\mathbf{k}) \pm \phi_2(\mathbf{k})]/\sqrt{2}$, in terms of which the eigenfunctions are

$$\phi^\pm(\mathbf{k}) = \cos\theta_{\mathbf{k}}\phi_{a,b}(\mathbf{k}) + i\sin\theta_{\mathbf{k}}\phi_{b,a}(\mathbf{k}), \quad (4)$$

with the phase factor $\theta_{\mathbf{k}} = \frac{1}{2}\arg(t_{12})$. At the zone center these wave functions have full bonding or antibonding character, which is exchanged at the $(\pi, \pi, 0)$ point. Elsewhere in the zone the character is mixed, except along the line $k_x = -k_y$, where the argument remains zero and a band crossing occurs. The nature of the eigenfunctions changes little with k_z , except close to $(\pi, \pi, 0)$ where there is another crossing. The two-band dispersion for a doping of $x = 0.15$ is illustrated in Fig. 2(a) for a \mathbf{k} -space path equivalent to that depicted in Refs. [11] and [3]. Although no crossings occur on this path, the character of the associated eigenfunctions is altered by evolution of the complex phase factor. The Fermi surfaces (Fig. 2(b)) for the two bands remain quasi-1d [3], in that they take the form of sheets crossed only along k_z , with some variation of k_{zF} depending on $\tilde{\mathbf{k}} \equiv (k_x, k_y)$.

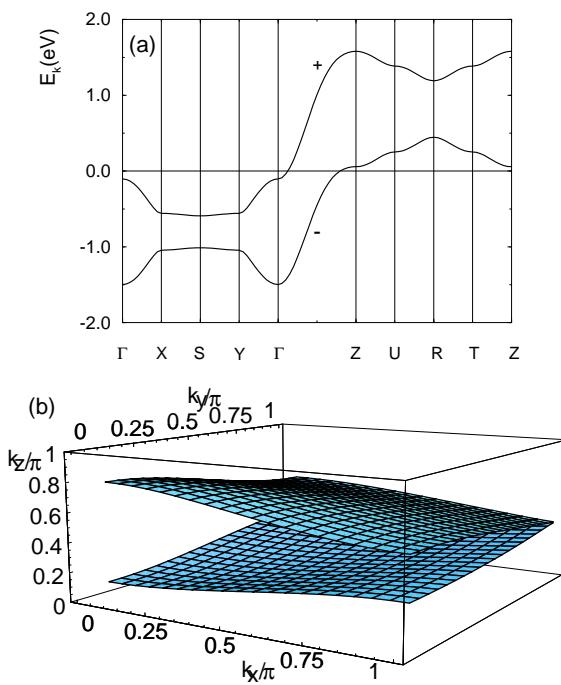


FIG. 2. (a) Tight-binding dispersion relations and (b) Fermi surfaces for two-band model at doping $x = 0.15$.

The gap equations describing superconductivity in a two-band system take the form

$$\Delta_{\mathbf{k}\alpha} = \frac{1}{V} \sum_{\mathbf{k}',\beta} V_{\mathbf{k}\mathbf{k}'\alpha\beta} \frac{\Delta_{\mathbf{k}'\beta}}{2E_{\mathbf{k}'\beta}} \tanh\left(\frac{E_{\mathbf{k}'\beta}}{2k_B T}\right), \quad (5)$$

where $\alpha, \beta = \pm$ are the band indices, $V_{\mathbf{k}\mathbf{k}'\alpha\beta}$ is a matrix containing both the on-site repulsion term and the pairing potential, and $E_{\mathbf{k}\alpha} = \pm\sqrt{(\epsilon_{\mathbf{k}\alpha} - \mu)^2 + \Delta_{\mathbf{k}\alpha}^2}$ specifies

the dispersion relations in the superconducting state (μ is the chemical potential). The symmetry of the gaps $\Delta_{\mathbf{k}\pm}$, both along (k_z) and transverse ($\tilde{\mathbf{k}}$) to the ladder axis, is of particular interest.

The pairing potential, as usual in cuprates, is repulsive. Scattering processes due to interactions with spin fluctuations should be strongly enhanced at the characteristic wave vector of the AF correlated ladder spins, $q_z = \pi$. The dominant contributions are expected from interband scattering of intraband electron pairs when the band separation is close to π , as represented schematically in Fig 3. To describe this we adopt the frequency-dependent MMP potential in the form

$$V_{\mathbf{k}\mathbf{k}'\alpha\beta} = \frac{-V_0 \epsilon_{\alpha\beta}}{\sqrt{(1 + \xi_z^2 |q_z - Q_z|^2)^2 + (\omega^2/\omega_{SF}^2)}}. \quad (6)$$

Here $q_z = k_z - k'_z$, $Q_z = \pi$ is the AF wave vector in the ladder direction, $\omega = \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}$ and ω_{SF} sets the frequency scale. $\epsilon_{\alpha\beta}$ is the off-diagonal tensor ensuring the interband scattering condition, and has the effect of a projector, $\sum_{m \neq n} |\phi_m\rangle\langle\phi_n|$, $m, n = a, b$, restricting the processes of interest to those scattering pairs between bonding and antibonding states. The longitudinal correlation length ξ_z determines the spin fluctuation enhancement, and may be deduced from the MMP parameters [10,12] for planar cuprate superconductors. We neglect the transverse dispersion of spin fluctuations: because [4,5] interladder superexchange is weak ($J_{\perp} \simeq 0.12J$), this would contribute an effect of order 10%, with the consequence that the leading components of any gap solution will be isotropic in $\tilde{\mathbf{k}}$.

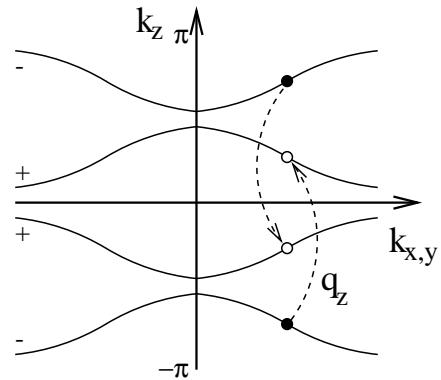


FIG. 3. Schematic Fermi-surface geometry showing important interband pair scattering processes.

The Hubbard-type model under consideration has also a repulsive on-site interaction U , which appears in the Hamiltonian as $H_U = \frac{1}{2}U \sum_{\mathbf{k}\alpha=\pm} (\Delta_{\mathbf{k}\alpha} c_{\mathbf{k}\uparrow}^{\alpha\dagger} c_{-\mathbf{k}\downarrow}^{\alpha\dagger} + H.c.)$. In the appropriate (t - J) limit of $U \rightarrow \infty$, the amplitude for pair creation on any site must be zero, which sets the constraint $\sum_{\mathbf{k}} c_{\mathbf{k}\uparrow}^{+\dagger} c_{-\mathbf{k}\downarrow}^{+\dagger} + c_{\mathbf{k}\uparrow}^{-\dagger} c_{-\mathbf{k}\downarrow}^{-\dagger} = 0$, or

$$\sum_{\mathbf{k}} \left[\frac{\Delta_{\mathbf{k}+}}{2E_{\mathbf{k}+}} + \frac{\Delta_{\mathbf{k}-}}{2E_{\mathbf{k}-}} \right] = 0. \quad (7)$$

The full, coupled gap equations can be written as

$$\Delta_{\mathbf{k}\alpha} = -\frac{1}{V} \sum_{\mathbf{k}'} \left[\frac{U}{2} D_{\mathbf{k}'\alpha} + \left(\frac{U}{2} + \frac{V_0}{B} \right) D_{\mathbf{k}'\bar{\alpha}} \right], \quad (8)$$

where

$$D_{\mathbf{k}\alpha} = \frac{\Delta_{\mathbf{k}\alpha}}{2E_{\mathbf{k}\alpha}} \tanh \left(\frac{E_{\mathbf{k}\alpha}}{2k_B T} \right), \quad (9)$$

$\alpha = \pm, \bar{\alpha} \equiv -\alpha$, and B denotes the denominator in Eq. (6). As both U and V terms are repulsive, the most straightforward solution is one where the gaps have opposite signs on the \pm bands. The symmetry of the U terms in D_+ and D_- ensures that the constraint (7) is obeyed.

We take the parameter values from planar cuprates [12], where the local physics can be expected to be similar. The correlation length is $\xi_z = 2.3a_c$. The prefactor is $V_0 = g^2 \chi_Q$, where $g = 1.53\text{eV}$ is the coefficient of the electron-spin fluctuation interaction and $\chi_Q = \pi(\xi/a)^2 \chi_0$ is a wave vector-adjusted static susceptibility; $\chi_0 = 2.62$ states/eV gives $V_0 \simeq 100$. The damping frequency is given by $\omega_{\text{SF}} = \Gamma/(\pi\xi/a)^2$, where $\Gamma = 0.4\text{eV}$ is the frequency cutoff of the interaction, whence $\omega_{\text{SF}} = 8\text{meV}$. The values of all parameters are taken to be constant at and below T_c . Considering the range of U , the constraint (7) is satisfied to within 1% for $U = 10J$, so this value is used below.

Solution of the gap equations (8) is simplified by separating the dependences of the pairing potential on k_z and $\tilde{\mathbf{k}}$, and a harmonic decomposition of the gap functions

$$\Delta_{\mathbf{k}}^{\pm} = \Delta_0^{\pm} + \Delta_1^{\pm} \cos k_z + \Delta_2^{\pm} \cos 2k_z + \dots \quad (10)$$

and the potential

$$V(\mathbf{k}, k_z) = \sum_{ij} V_{ij}(\tilde{\mathbf{k}}) \cos ik_z \cos jk_z. \quad (11)$$

The dominant contributions to $V_{ij}(\tilde{\mathbf{k}})$ are from Fermi-surface scattering processes with $\epsilon_{\mathbf{k}} = 0$. The approximate treatment is justified by the parameters ξ_z and ω_{SF} , which are such that the halfwidth of $V(q_z)$ is $\delta q \sim 0.2\pi$, a quantity exceeding the variation in band separation $k_{zF}^+ - k_{zF}^-$ across the Brillouin zone (Fig. 2(b)). Thus scattering vectors of all $\tilde{\mathbf{q}}$ contribute similarly, and the averaging performed in the approximation introduces insignificant errors.

The qualitative nature of the solutions is influenced by the doping. In this treatment the band shape is not affected, but a change of doping alters the separation of the Fermi surfaces (Fig. 3). The pairing is (broadly) peaked where the bands have maximal areas separated by $q_z \simeq \pi$.

We find that at $x_m = 0.112$ the separation is π at $\tilde{\mathbf{k}} = (0,0)$, and is smaller than π everywhere else in the zone. Increased doping ($x > x_m$) causes the net interaction to diminish, while at $x < x_m$ a circle of band separation π will open and increase in circumference, implying a monotonic rise in any T_c , at least until $x = 0.082$ where Fermi surface is lost to formation of an electron pocket at Z in the $-$ band. We have solved the gap equations for a variety of doping values $0.05 < x < 0.2$, retaining interaction coefficients V_{ij} up to fourth order, and gap components Δ_i to $i = 2$.

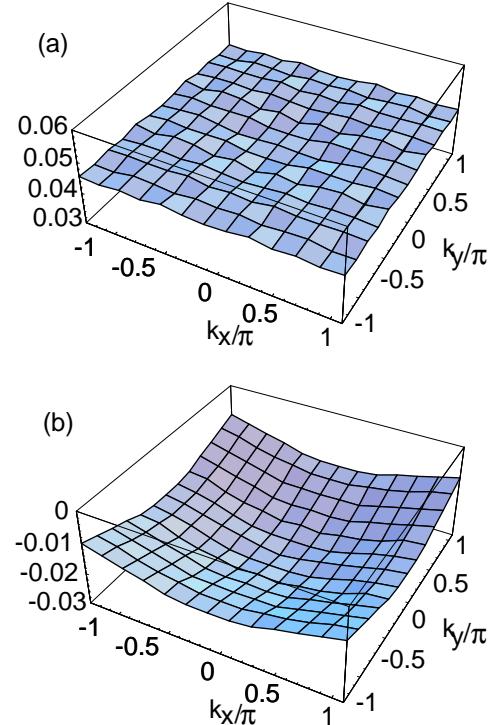


FIG. 4. Superconducting gaps (a) $\Delta_{\mathbf{k}}^+$ and (b) $\Delta_{\mathbf{k}}^-$ on the Fermi surfaces for doping $x = 0.082$.

A superconducting solution with finite gap components is obtained for all the doping levels considered. The gaps have opposite signs, and no nodes. Figs. 4(a) and (b) show these full gaps on the Fermi surfaces for doping $x = 0.082$, which is qualitatively representative of all cases. $\Delta_{\mathbf{k}}^+$ is effectively constant, while $\Delta_{\mathbf{k}}^-$ has only appreciable zeroth and first harmonics, justifying the neglect of higher components. That the order parameters have opposite signs on each band corresponds within the ladder to the condition [13] for “*d*-like” symmetry that $\Delta(k_{\perp} = 0)$ and $\Delta(k_{\perp} = \pi)$ have opposite signs. The order parameters are isotropic transverse to the ladder direction. The decrease of gap components with doping is quantified by T_c (Fig. 5). The slower increase with decreasing doping below $x = 0.082$ may be accounted for as above. Quantitatively, the values of T_c predicted from the

two-band model with spin fluctuation-mediated pairing approach those of the 2d planar cuprate $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

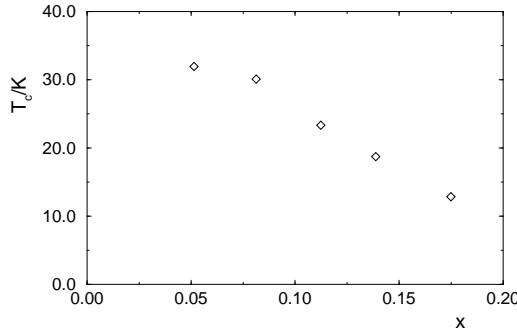


FIG. 5. T_c as a function of doping for two-band model.

Our primary result is then that, within a specific model for AF spin fluctuations, the coupled ladder compound $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$ is predicted to be superconducting. Since the solutions of the gap equations have a full gap over the whole Fermi surface with opposite signs on the different sheets, there is clearly no inherent frustration for a superconductor with approximate d -wave symmetry. From this point of view, it appears rather that the Fermi surface form would favor a superconducting state. The primary weakness of the preceding calculation is that it is carried out for a clean system, whereas in reality there are two sources of disorder. One is crystalline imperfections, which presumably may be controlled, and the other is intrinsic to the doping process which substitutes divalent Sr^{2+} ions for trivalent La^{3+} in close proximity to the ladders. Evidence for the disruptive influence of this random potential may be found in recent experiments on thin films of $\text{La}_{1.9}\text{Sr}_{0.1}\text{CuO}_4$ [14], in which the distance of Sr^{2+} from the cuprate planes was varied. For greater separation, the transition temperature was substantially enhanced, from 29K to $T_c = 50\text{K}$, and simultaneously the in-plane resistivity in the normal state was reduced. This source of disorder cannot be eliminated, and may lead to localization, particularly at lower x , which would produce a doping dependence of T_c of the type manifest in the planar cuprates (*cf.* Fig. 5). The synthesis of crystalline samples with $x = 0.15$ and low residual resistivities [7] is encouraging in the following regard. It provides hope that if high-quality single crystals could be synthesized for smaller x , there is the possibility of superconductivity, or at minimum of the observation of spin-gap features similar to the underdoped cuprates. If in the latter case a crossover to an insulating phase appeared at low temperatures, this would be *prime facie* evidence that indeed the presence of disorder was responsible for a suppression of superconductivity.

A related question concerns the Landau Fermi liquid nature of the metallic state observed at $x = 0.15$. At first sight, the quasi-1d nature of $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$ should ac-

celerate the breakdown of Landau theory, yet it seems that the critical doping required to stabilize it is actually lower than in the planar cuprates. One possible explanation for this unexpected discrepancy is the role of Umklapp scattering, which has been proposed [15] as the cause of the breakdown of Landau behavior in 2d cuprate systems. In the present case, Umklapp scattering between the two Fermi-surface sheets occurs only for smaller values of $x \leq x_m = 0.112$. Again it would be most interesting to follow the evolution of the normal state in samples with lower doping.

In conclusion, we have found that from the point of view of spin-fluctuation theory, the $\text{La}_{1-x}\text{Sr}_x\text{CuO}_{2.5}$ system, with its clear ladder structure, should favor a nodeless, d -wave superconducting state. However, this may be suppressed by the strong intrinsic disorder introduced by substituting Sr^{2+} for La^{3+} . The synthesis of crystalline samples with low doping values would shed light on many key issues in the understanding of cuprates.

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